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First-Principles Calculations of Palladium Nanostructures Formed on γ-Alumina[1] XIN LIU, SANWU WANG, The University of Tulsa — Palladium clusters supported on the γ-alumina surface serve as a catalyst for a variety of important chemical reactions. We report results of our first-principles quantum mechanical calculations for the bonding configurations of palladium atoms and clusters that are supported on the γ-Al_2O_3(110) surface. In particular, our results show that while a single Pd atom prefers to be bonded on the bridge sites of two surface aluminum atoms, a chain nanostructure and a ring-like nanostructure may be formed when more Pd atoms are adsorbed on the surface.

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